



# Full wwPDB X-ray Structure Validation Report

Nov 20, 2014 – 07:02 PM EST

PDB ID : 4V0O  
Title : Crystal structure of BBS1N in complex with ARL6DN, soaked with lead  
Authors : Mourao, A.; Lorentzen, E.  
Deposited on : 2014-09-17  
Resolution : 3.35 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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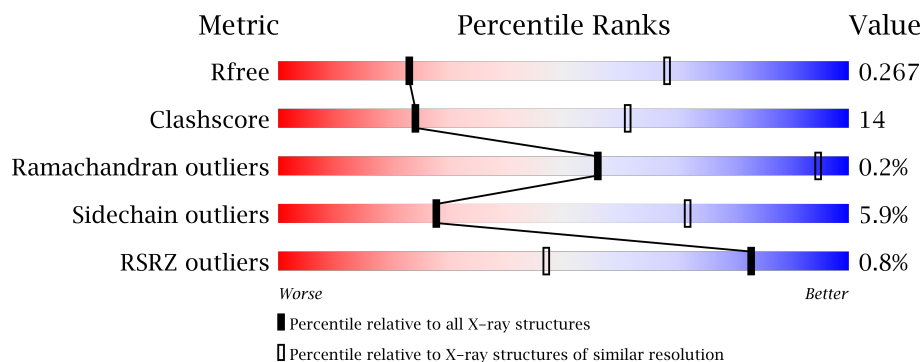
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24195  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24195

# 1 Overall quality at a glance

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1141 (3.50-3.22)
Clashscore	79885	1030 (3.48-3.24)
Ramachandran outliers	78287	1008 (3.48-3.24)
Sidechain outliers	78261	1007 (3.48-3.24)
RSRZ outliers	66119	1141 (3.50-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	169	
1	C	169	
1	E	169	
1	G	169	
2	B	425	
2	D	425	
2	F	425	
2	H	425	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14519 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ARF-LIKE SMALL GTPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1265	809	215	235	6			
1	C	166	Total	C	N	O	S	0	0	0
			1291	823	223	239	6			
1	E	166	Total	C	N	O	S	0	0	0
			1278	816	219	237	6			
1	G	166	Total	C	N	O	S	0	0	0
			1286	822	221	237	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	EXPRESSION TAG	UNP A8JF99
A	13	ALA	-	EXPRESSION TAG	UNP A8JF99
A	14	ALA	-	EXPRESSION TAG	UNP A8JF99
A	15	SER	-	EXPRESSION TAG	UNP A8JF99
C	12	GLY	-	EXPRESSION TAG	UNP A8JF99
C	13	ALA	-	EXPRESSION TAG	UNP A8JF99
C	14	ALA	-	EXPRESSION TAG	UNP A8JF99
C	15	SER	-	EXPRESSION TAG	UNP A8JF99
E	12	GLY	-	EXPRESSION TAG	UNP A8JF99
E	13	ALA	-	EXPRESSION TAG	UNP A8JF99
E	14	ALA	-	EXPRESSION TAG	UNP A8JF99
E	15	SER	-	EXPRESSION TAG	UNP A8JF99
G	12	GLY	-	EXPRESSION TAG	UNP A8JF99
G	13	ALA	-	EXPRESSION TAG	UNP A8JF99
G	14	ALA	-	EXPRESSION TAG	UNP A8JF99
G	15	SER	-	EXPRESSION TAG	UNP A8JF99

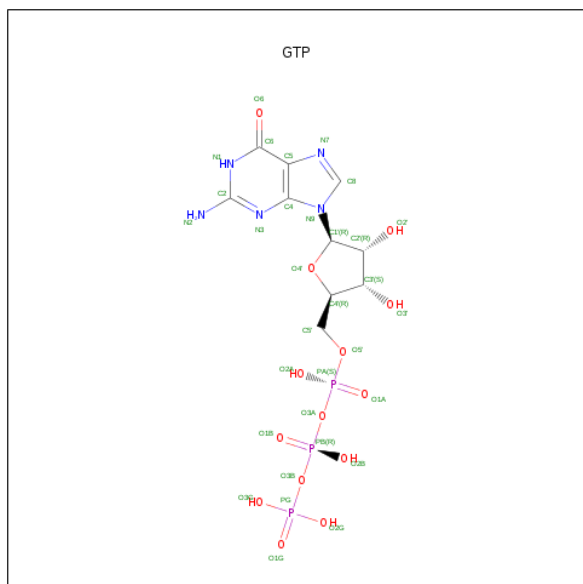
- Molecule 2 is a protein called BARDET-BIEDL SYNDROME 1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	333	Total	C	N	O	S	0	0	0
			2428	1551	422	442	13			
2	D	307	Total	C	N	O	S	0	0	0
			2205	1401	387	405	12			
2	F	309	Total	C	N	O	S	0	0	0
			2230	1424	384	409	13			
2	H	325	Total	C	N	O	S	0	0	0
			2386	1525	411	437	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ARG	LYS	CONFLICT	UNP A8JEA1
D	37	ARG	LYS	CONFLICT	UNP A8JEA1
F	37	ARG	LYS	CONFLICT	UNP A8JEA1
H	37	ARG	LYS	CONFLICT	UNP A8JEA1

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

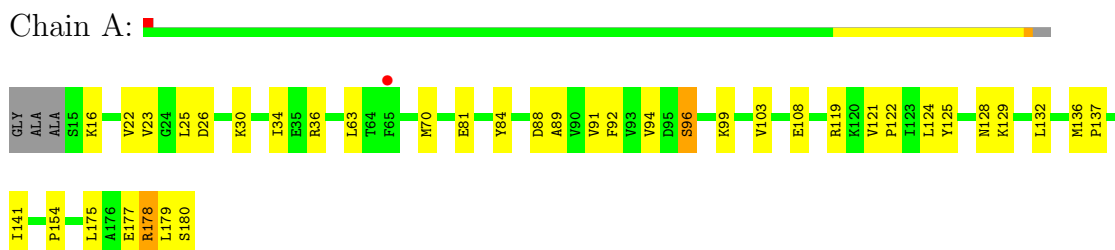
- Molecule 5 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Pb	0	0
			1	1		
5	D	3	Total	Pb	0	0
			3	3		
5	E	1	Total	Pb	0	0
			1	1		
5	H	4	Total	Pb	0	0
			4	4		
5	B	4	Total	Pb	0	0
			4	4		
5	A	2	Total	Pb	0	0
			2	2		
5	F	3	Total	Pb	0	0
			3	3		

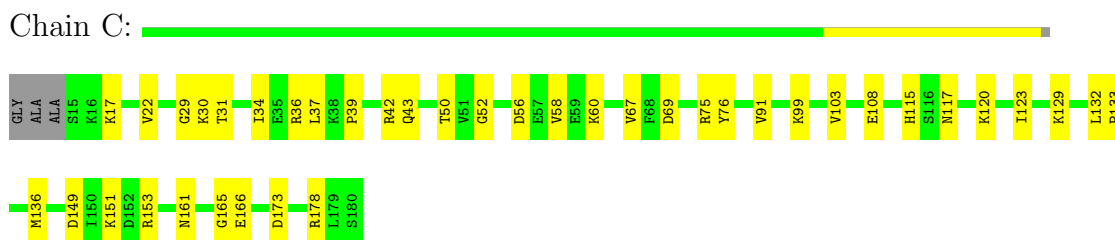
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

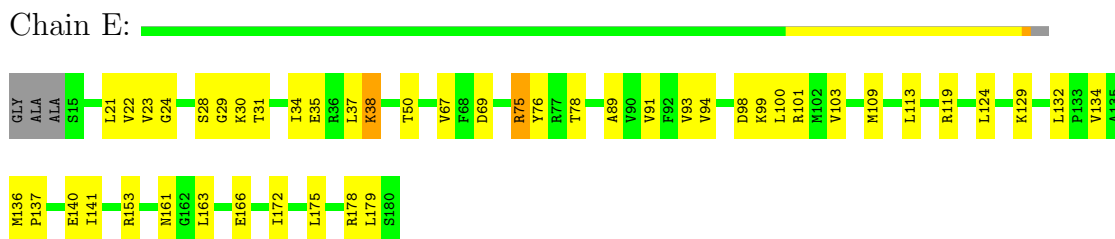
- Molecule 1: ARF-LIKE SMALL GTPASE



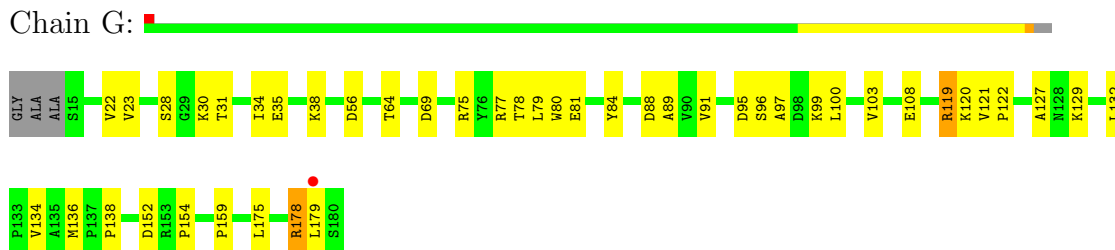
- Molecule 1: ARF-LIKE SMALL GTPASE



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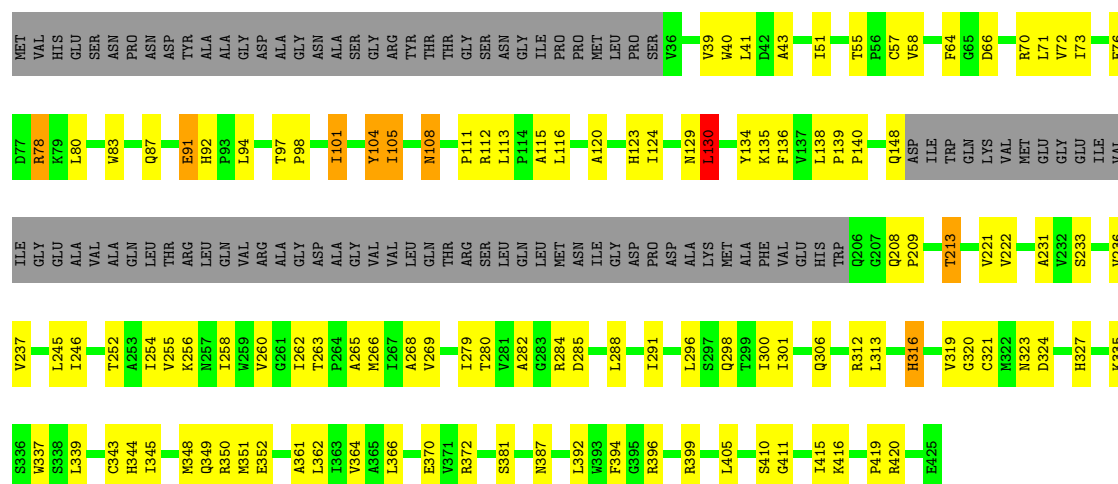


- Molecule 1: ARF-LIKE SMALL GTPASE



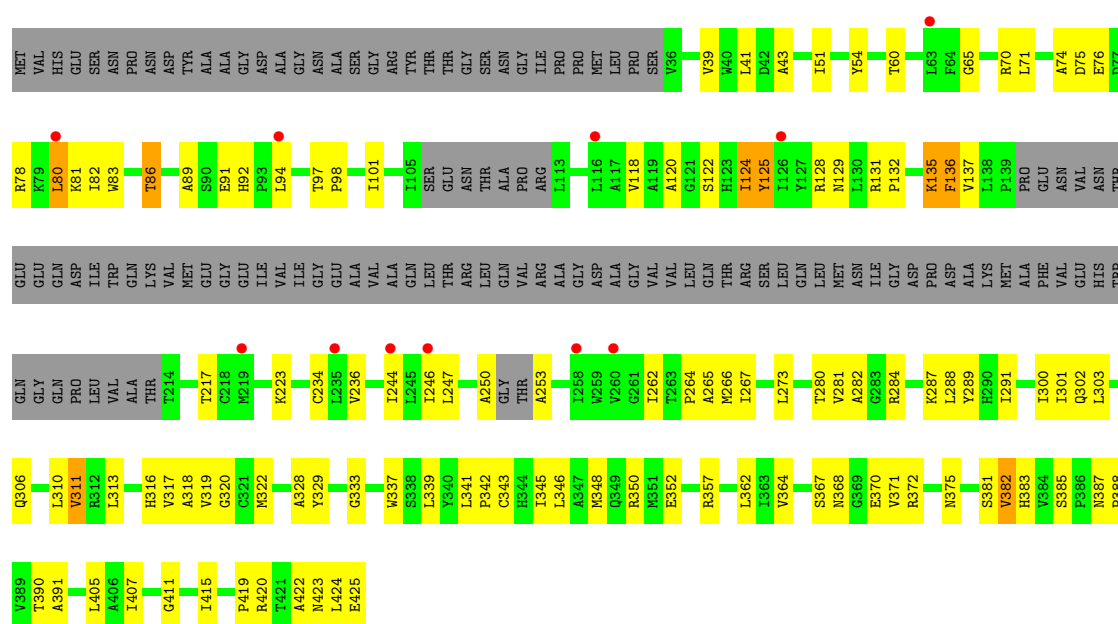
- Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

## Chain B:



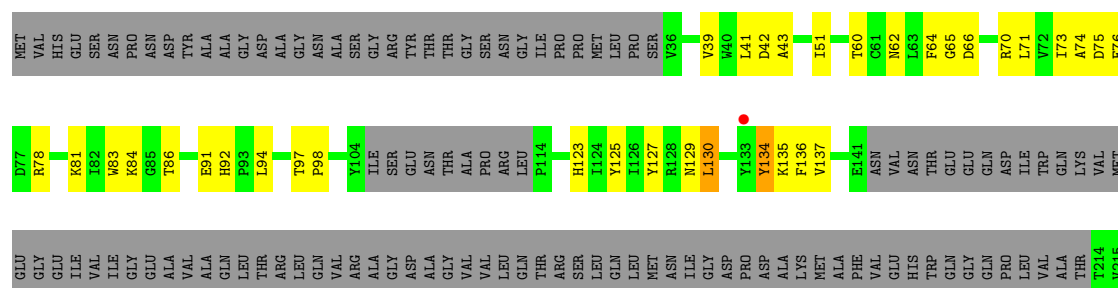
## • Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

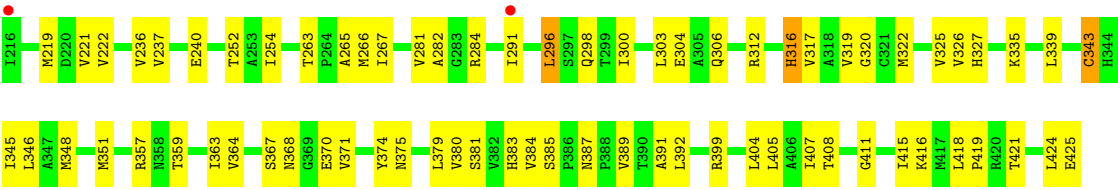
## Chain D:



## • Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

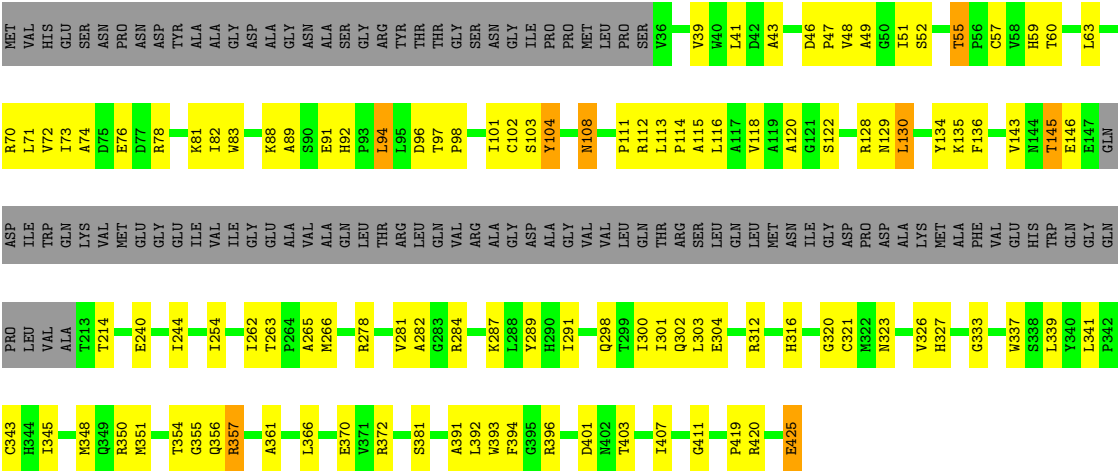
## Chain F:





● Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

Chain H:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.70Å 123.70Å 439.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	96.27 – 3.35 96.27 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (96.27-3.35) 99.3 (96.27-3.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.221 , 0.268 0.219 , 0.267	Depositor DCC
$R_{free}$ test set	2839 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	114.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , -0.7	EDS
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 56809 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, PB, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/1291	0.65	0/1758
1	C	0.65	0/1317	0.77	0/1788
1	E	0.65	0/1304	0.78	0/1773
1	G	0.49	0/1312	0.67	0/1781
2	B	0.59	0/2480	0.79	2/3398 (0.1%)
2	D	0.47	0/2247	0.71	1/3077 (0.0%)
2	F	0.50	0/2276	0.73	0/3118
2	H	0.57	0/2437	0.78	1/3341 (0.0%)
All	All	0.55	0/14664	0.74	4/20034 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	356	GLN	N-CA-C	-7.27	91.38	111.00
2	B	130	LEU	CA-CB-CG	5.37	127.66	115.30
2	D	80	LEU	CA-CB-CG	5.37	127.65	115.30
2	B	208	GLN	N-CA-C	5.17	124.95	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	355	GLY	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1265	0	1248	25	0
1	C	1291	0	1297	34	0
1	E	1278	0	1272	36	0
1	G	1286	0	1294	30	0
2	B	2428	0	2359	74	0
2	D	2205	0	2101	72	0
2	F	2230	0	2145	70	0
2	H	2386	0	2329	79	0
3	A	32	0	12	4	0
3	C	32	0	12	3	0
3	E	32	0	12	5	0
3	G	32	0	12	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
5	D	3	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	1	0
5	G	1	0	0	0	0
5	H	4	0	0	0	0
All	All	14519	0	14093	405	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (405) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:129:LYS:HB3	1:C:132:LEU:HD12	1.58	0.84
2:D:82:ILE:HG22	2:D:89:ALA:HB3	1.64	0.80
2:D:74:ALA:HB1	2:D:98:PRO:HG2	1.63	0.79
2:F:39:VAL:HG13	2:F:381:SER:HB2	1.64	0.79
2:F:91:GLU:O	2:F:92:HIS:ND1	2.17	0.78
2:B:350:ARG:NH2	2:B:352:GLU:OE1	2.16	0.78
2:H:112:ARG:N	2:H:113:LEU:HA	1.99	0.77
2:D:39:VAL:HG13	2:D:381:SER:HB2	1.66	0.77
1:G:129:LYS:HB3	1:G:132:LEU:HD12	1.67	0.76
2:H:72:VAL:HG11	2:H:116:LEU:HD11	1.67	0.75
1:G:99:LYS:HA	1:G:136:MET:HE1	1.68	0.75
1:E:129:LYS:HB3	1:E:132:LEU:HD12	1.70	0.73
2:B:41:LEU:HG	2:B:419:PRO:HG3	1.71	0.73
2:H:136:PHE:HZ	2:H:254:ILE:HG13	1.54	0.72
1:C:30:LYS:O	1:C:34:ILE:HG13	1.89	0.72
1:G:89:ALA:HB2	1:G:179:LEU:HD21	1.72	0.72
2:D:91:GLU:O	2:D:92:HIS:ND1	2.21	0.71
2:H:91:GLU:O	2:H:92:HIS:ND1	2.24	0.71
2:D:311:VAL:HG11	2:D:362:LEU:HD13	1.73	0.70
2:D:94:LEU:HD13	2:D:98:PRO:HG3	1.74	0.70
2:H:94:LEU:HD22	2:H:98:PRO:HG3	1.74	0.69
2:D:346:LEU:HD21	2:D:367:SER:HB3	1.75	0.69
1:A:108:GLU:OE2	2:B:420:ARG:NH1	2.26	0.69
2:H:39:VAL:HG13	2:H:381:SER:HB2	1.75	0.68
2:B:136:PHE:HE2	2:B:138:LEU:HD23	1.57	0.68
2:B:112:ARG:N	2:B:113:LEU:HA	2.08	0.68
2:B:71:LEU:HB3	2:B:83:TRP:HB2	1.75	0.68
1:C:103:VAL:HG11	2:D:43:ALA:HA	1.75	0.68
2:H:108:ASN:OD1	2:H:108:ASN:N	2.26	0.68
2:D:348:MET:HG2	2:D:364:VAL:HG12	1.76	0.68
2:F:296:LEU:HD23	2:F:296:LEU:H	1.59	0.68
2:B:265:ALA:HB2	2:B:284:ARG:HG2	1.76	0.67
2:H:341:LEU:HD23	2:H:366:LEU:HD11	1.77	0.67
2:B:72:VAL:HG11	2:B:116:LEU:HD11	1.77	0.66
2:F:71:LEU:HB3	2:F:83:TRP:HB2	1.77	0.66
2:F:42:ASP:OD1	2:F:416:LYS:NZ	2.27	0.66
1:C:30:LYS:N	3:C:600:GTP:O1B	2.21	0.66
1:A:129:LYS:HB3	1:A:132:LEU:HD12	1.77	0.66
2:H:55:THR:HG23	2:H:392:LEU:H	1.61	0.66
1:A:129:LYS:HG2	3:A:600:GTP:C6	2.30	0.66
2:H:94:LEU:HD21	2:H:118:VAL:HG11	1.78	0.65
2:D:266:MET:HG3	2:D:310:LEU:HB3	1.78	0.65
2:H:130:LEU:O	2:H:130:LEU:HG	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:51:ILE:HD13	2:B:73:ILE:HD13	1.78	0.65
2:B:321:CYS:HB2	2:B:323:ASN:OD1	1.97	0.65
1:C:39:PRO:HD2	1:C:42:ARG:HD2	1.79	0.65
2:H:51:ILE:HD13	2:H:73:ILE:HD13	1.79	0.65
2:B:288:LEU:HD11	2:B:319:VAL:HG21	1.79	0.64
2:D:265:ALA:HB2	2:D:284:ARG:HG2	1.78	0.64
2:F:346:LEU:HD21	2:F:367:SER:HB3	1.79	0.64
1:E:89:ALA:HB1	1:E:175:LEU:HD11	1.80	0.64
2:F:134:TYR:HD1	2:F:135:LYS:H	1.45	0.63
1:E:30:LYS:N	3:E:600:GTP:O1B	2.21	0.63
2:B:134:TYR:CZ	2:B:252:THR:HG23	2.34	0.63
2:D:350:ARG:NH2	2:D:352:GLU:OE1	2.32	0.62
1:G:103:VAL:HG11	2:H:43:ALA:HA	1.82	0.61
2:F:304:GLU:OE2	2:F:327:HIS:NE2	2.22	0.61
1:G:178:ARG:HH11	1:G:178:ARG:N	1.99	0.61
1:G:108:GLU:OE1	2:H:420:ARG:NH1	2.34	0.61
2:B:104:TYR:CE1	2:B:115:ALA:HB3	2.37	0.60
2:B:91:GLU:O	2:B:92:HIS:ND1	2.34	0.60
2:F:123:HIS:HA	2:F:137:VAL:HG22	1.82	0.60
1:A:22:VAL:HG22	1:A:91:VAL:HB	1.84	0.60
1:A:30:LYS:NZ	1:A:70:MET:O	2.35	0.60
2:H:244:ILE:HD11	2:H:281:VAL:HG21	1.83	0.60
1:G:81:GLU:HA	1:G:84:TYR:CD2	2.37	0.59
2:B:222:VAL:HG23	2:B:236:VAL:HG21	1.84	0.59
2:H:41:LEU:HG	2:H:419:PRO:HG3	1.83	0.59
1:E:99:LYS:HA	1:E:136:MET:HE1	1.83	0.59
2:F:134:TYR:HE2	2:F:252:THR:HA	1.66	0.59
2:F:418:LEU:HD12	2:F:419:PRO:HD2	1.85	0.59
2:F:74:ALA:HB1	2:F:98:PRO:HG2	1.83	0.59
3:A:600:GTP:C8	3:A:600:GTP:H5'	2.37	0.59
2:D:236:VAL:HG22	2:D:246:ILE:HG23	1.84	0.59
2:H:60:THR:HG22	2:H:71:LEU:HA	1.85	0.58
2:F:125:TYR:CD1	2:F:135:LYS:HG2	2.39	0.58
2:D:368:ASN:OD1	2:D:370:GLU:HG2	2.04	0.58
2:B:255:VAL:HG12	2:B:256:LYS:HG2	1.84	0.58
2:B:262:ILE:HG12	2:B:285:ASP:HB3	1.85	0.58
1:A:16:LYS:HB3	1:A:63:LEU:HD23	1.84	0.58
2:B:51:ILE:O	2:B:411:GLY:HA2	2.03	0.58
1:A:96:SER:HB2	1:A:128:ASN:O	2.03	0.57
1:E:103:VAL:HG22	2:F:41:LEU:HD13	1.85	0.57
2:H:266:MET:HG2	2:H:282:ALA:HB3	1.86	0.57
2:D:345:ILE:HG21	2:D:348:MET:HE2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:94:LEU:HD13	2:F:98:PRO:HG3	1.85	0.57
2:H:49:ALA:HB1	2:H:51:ILE:HG13	1.85	0.57
1:C:99:LYS:HB3	2:D:86:THR:HG21	1.86	0.57
2:H:104:TYR:CE1	2:H:115:ALA:HB3	2.39	0.57
2:B:108:ASN:N	2:B:108:ASN:OD1	2.28	0.57
2:H:136:PHE:CZ	2:H:254:ILE:HG13	2.38	0.57
1:E:37:LEU:HD21	1:E:172:ILE:HG13	1.86	0.57
2:F:70:ARG:HH11	2:F:84:LYS:CB	2.17	0.57
1:C:129:LYS:HG2	3:C:600:GTP:C6	2.40	0.56
1:G:38:LYS:HE2	1:G:56:ASP:OD2	2.05	0.56
1:C:123:ILE:HD11	1:C:153:ARG:HD3	1.86	0.56
2:D:267:ILE:HG22	2:D:281:VAL:HG22	1.88	0.56
1:G:89:ALA:HB1	1:G:175:LEU:HD11	1.87	0.56
2:D:391:ALA:HB3	2:D:407:ILE:HB	1.88	0.56
2:F:368:ASN:OD1	2:F:370:GLU:HG2	2.05	0.56
2:F:222:VAL:HG23	2:F:236:VAL:HG21	1.87	0.56
2:B:98:PRO:HA	2:B:120:ALA:HB2	1.88	0.56
2:D:54:TYR:CD2	2:D:390:THR:HB	2.41	0.56
2:H:63:LEU:HD21	2:H:116:LEU:HD12	1.89	0.55
2:H:122:SER:HB3	2:H:214:THR:O	2.06	0.55
2:D:423:ASN:N	2:D:423:ASN:OD1	2.39	0.55
2:H:370:GLU:OE2	2:H:372:ARG:NE	2.38	0.55
2:F:343:CYS:HB2	2:F:368:ASN:ND2	2.20	0.55
2:F:75:ASP:OD2	2:F:81:LYS:HE3	2.07	0.55
2:B:279:ILE:HB	2:B:291:ILE:HB	1.89	0.55
2:D:250:ALA:O	2:D:253:ALA:N	2.40	0.55
1:E:31:THR:OG1	3:E:600:GTP:O2B	2.24	0.55
1:C:103:VAL:HG22	2:D:41:LEU:HD13	1.89	0.54
2:H:51:ILE:O	2:H:411:GLY:HA2	2.08	0.54
2:D:357:ARG:NH1	2:D:422:ALA:O	2.34	0.54
2:H:321:CYS:HB2	2:H:323:ASN:OD1	2.06	0.54
3:G:600:GTP:H5'	3:G:600:GTP:H8	1.73	0.54
2:H:101:ILE:HD12	2:H:116:LEU:HD21	1.90	0.54
1:C:120:LYS:HA	1:C:153:ARG:NH1	2.23	0.54
2:F:357:ARG:O	2:F:359:THR:HG23	2.08	0.54
2:H:71:LEU:HB3	2:H:83:TRP:HB2	1.89	0.54
1:C:36:ARG:NH1	1:C:43:GLN:OE1	2.41	0.53
2:H:351:MET:HA	2:H:394:PHE:CD2	2.43	0.53
2:D:125:TYR:CD1	2:D:135:LYS:HD3	2.43	0.53
2:D:41:LEU:HG	2:D:419:PRO:HG3	1.91	0.53
1:E:29:GLY:N	3:E:600:GTP:O1B	2.40	0.53
1:G:22:VAL:HG22	1:G:91:VAL:HB	1.89	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:129:ASN:N	2:F:130:LEU:HA	2.23	0.53
2:B:64:PHE:HB2	2:B:66:ASP:OD1	2.08	0.53
2:F:326:VAL:HB	2:F:339:LEU:HB2	1.90	0.53
2:B:320:GLY:HA3	2:B:348:MET:CE	2.40	0.52
2:B:80:LEU:HB2	2:B:94:LEU:HD13	1.90	0.52
1:E:75:ARG:CZ	1:E:76:TYR:HE1	2.22	0.52
2:F:265:ALA:HB2	2:F:284:ARG:HG2	1.92	0.52
2:H:304:GLU:OE2	2:H:327:HIS:NE2	2.42	0.52
1:G:122:PRO:HA	1:G:154:PRO:HG2	1.91	0.52
2:B:351:MET:HG3	2:B:394:PHE:CE2	2.45	0.52
2:H:345:ILE:HG21	2:H:348:MET:HE2	1.92	0.52
1:A:23:VAL:HG23	1:A:92:PHE:CD2	2.45	0.52
2:B:298:GLN:O	2:B:300:ILE:HD12	2.10	0.52
1:A:103:VAL:HG11	2:B:43:ALA:HA	1.91	0.52
2:H:76:GLU:C	2:H:78:ARG:H	2.13	0.52
2:B:266:MET:HG2	2:B:282:ALA:HB3	1.91	0.51
2:D:217:THR:OG1	2:D:264:PRO:HG2	2.10	0.51
2:B:101:ILE:HD12	2:B:116:LEU:HD21	1.93	0.51
2:B:39:VAL:HG13	2:B:381:SER:HB2	1.92	0.51
2:D:98:PRO:HA	2:D:120:ALA:HB2	1.91	0.51
2:D:244:ILE:HD11	2:D:281:VAL:HG21	1.93	0.51
1:E:34:ILE:HD13	1:E:67:VAL:HG11	1.91	0.51
2:D:54:TYR:CE2	2:D:390:THR:HB	2.46	0.51
1:A:89:ALA:HB1	1:A:175:LEU:HD11	1.93	0.51
2:H:129:ASN:N	2:H:130:LEU:HA	2.25	0.51
2:H:337:TRP:CE3	2:H:339:LEU:HD13	2.46	0.51
2:H:60:THR:HG1	2:H:393:TRP:HE1	1.59	0.51
2:B:105:ILE:HG12	2:B:231:ALA:O	2.11	0.51
3:G:600:GTP:C8	3:G:600:GTP:H5'	2.46	0.51
2:D:311:VAL:HG12	2:D:318:ALA:HB3	1.92	0.50
2:D:51:ILE:O	2:D:411:GLY:HA2	2.10	0.50
1:A:89:ALA:HB2	1:A:179:LEU:HD21	1.93	0.50
3:A:600:GTP:H8	3:A:600:GTP:H5'	1.76	0.50
1:E:29:GLY:HA2	3:E:600:GTP:O1A	2.11	0.50
1:E:98:ASP:OD2	1:E:101:ARG:HG3	2.12	0.50
2:D:101:ILE:HG22	2:D:118:VAL:HA	1.93	0.50
2:F:75:ASP:OD1	2:F:76:GLU:N	2.45	0.50
2:F:348:MET:HG2	2:F:364:VAL:HG12	1.94	0.50
2:B:362:LEU:HD22	2:B:364:VAL:HG23	1.93	0.49
2:B:94:LEU:HD23	2:B:98:PRO:HG3	1.94	0.49
2:F:312:ARG:HG3	2:F:312:ARG:O	2.12	0.49
2:F:60:THR:HG22	2:F:71:LEU:HA	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:278:ARG:HA	2:H:291:ILE:O	2.12	0.49
2:F:371:VAL:HB	2:F:383:HIS:NE2	2.28	0.49
2:B:370:GLU:OE1	2:B:372:ARG:NE	2.44	0.49
1:C:99:LYS:HG3	1:C:136:MET:SD	2.52	0.49
1:E:161:ASN:HB3	1:E:166:GLU:HB3	1.95	0.49
1:E:31:THR:HG23	1:E:69:ASP:OD2	2.11	0.49
1:C:149:ASP:HA	1:C:151:LYS:HE3	1.94	0.49
2:H:74:ALA:HB1	2:H:98:PRO:HG2	1.94	0.49
1:E:30:LYS:O	1:E:34:ILE:HG13	2.13	0.49
2:F:43:ALA:HB3	2:F:415:ILE:O	2.12	0.49
1:G:96:SER:O	1:G:136:MET:N	2.43	0.49
2:D:423:ASN:ND2	2:D:425:GLU:OE2	2.46	0.49
2:H:320:GLY:HA3	2:H:348:MET:CE	2.43	0.49
1:A:99:LYS:HA	1:A:136:MET:HE1	1.94	0.49
2:F:391:ALA:HB3	2:F:407:ILE:HB	1.95	0.49
2:D:371:VAL:HB	2:D:383:HIS:NE2	2.28	0.49
2:D:375:ASN:ND2	2:D:424:LEU:O	2.44	0.49
2:D:75:ASP:OD2	2:D:81:LYS:HE3	2.13	0.49
2:F:327:HIS:CE1	2:F:335:LYS:HE3	2.48	0.49
2:H:298:GLN:O	2:H:300:ILE:HD12	2.13	0.49
2:H:396:ARG:NH1	2:H:401:ASP:OD1	2.46	0.49
2:B:136:PHE:CE2	2:B:138:LEU:HD23	2.44	0.48
2:D:287:LYS:HE2	2:D:302:GLN:OE1	2.13	0.48
2:B:260:VAL:HG22	2:B:296:LEU:HG	1.96	0.48
2:F:51:ILE:O	2:F:411:GLY:HA2	2.13	0.48
2:F:266:MET:HG2	2:F:282:ALA:HB3	1.95	0.48
1:A:88:ASP:O	1:A:121:VAL:HB	2.12	0.48
2:B:108:ASN:O	2:B:111:PRO:HD3	2.13	0.48
2:D:136:PHE:CZ	2:D:253:ALA:HA	2.48	0.48
2:D:385:SER:OG	2:D:387:ASN:O	2.31	0.48
2:B:345:ILE:HG21	2:B:348:MET:HE2	1.94	0.48
2:B:350:ARG:NH2	2:B:352:GLU:HB2	2.28	0.48
2:F:136:PHE:HZ	2:F:254:ILE:HG13	1.77	0.48
1:E:31:THR:OG1	1:E:50:THR:OG1	2.31	0.48
2:H:287:LYS:HE2	2:H:302:GLN:OE1	2.13	0.48
1:A:30:LYS:O	1:A:34:ILE:HG13	2.14	0.48
1:E:24:GLY:O	1:E:30:LYS:HE2	2.14	0.48
1:G:127:ALA:HB3	1:G:159:PRO:HA	1.96	0.48
2:D:328:ALA:HB3	2:D:337:TRP:H	1.79	0.48
2:H:94:LEU:HD11	2:H:118:VAL:HG21	1.95	0.48
2:B:123:HIS:CE1	2:B:135:LYS:HD3	2.49	0.47
2:H:262:ILE:HD12	2:H:263:THR:H	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:35:GLU:HA	1:E:38:LYS:HD3	1.97	0.47
2:F:375:ASN:ND2	2:F:424:LEU:O	2.38	0.47
2:B:111:PRO:HB2	2:B:113:LEU:CB	2.44	0.47
1:G:23:VAL:HB	1:G:80:TRP:CZ3	2.50	0.47
2:D:346:LEU:HD11	2:D:388:PRO:HB2	1.97	0.47
2:F:76:GLU:C	2:F:78:ARG:H	2.16	0.47
2:B:129:ASN:N	2:B:130:LEU:HA	2.29	0.47
2:B:76:GLU:C	2:B:78:ARG:H	2.17	0.47
2:H:425:GLU:N	2:H:425:GLU:OE1	2.48	0.47
2:B:130:LEU:O	2:B:130:LEU:HG	2.13	0.47
2:D:125:TYR:HD1	2:D:135:LYS:HD3	1.78	0.47
2:F:240:GLU:HG3	2:F:263:THR:HG23	1.96	0.47
1:G:120:LYS:HD2	1:G:152:ASP:HB2	1.97	0.47
2:H:351:MET:HG3	2:H:394:PHE:CE2	2.49	0.47
2:H:41:LEU:CG	2:H:419:PRO:HG3	2.45	0.47
2:F:51:ILE:HD13	2:F:73:ILE:HD13	1.96	0.47
2:H:82:ILE:HG22	2:H:89:ALA:HB3	1.97	0.47
2:B:140:PRO:HB3	2:B:213:THR:HG23	1.97	0.47
2:D:289:TYR:CD1	2:D:300:ILE:HD12	2.49	0.47
2:F:320:GLY:HA3	2:F:348:MET:CE	2.45	0.47
1:G:35:GLU:OE1	1:G:38:LYS:HD2	2.14	0.47
1:C:39:PRO:HG2	1:C:42:ARG:CZ	2.45	0.47
1:E:34:ILE:HD13	1:E:67:VAL:CG1	2.45	0.47
2:F:387:ASN:HB2	2:F:408:THR:HB	1.97	0.46
2:H:394:PHE:HA	2:H:403:THR:O	2.15	0.46
2:H:59:HIS:CE1	2:H:103:SER:HB3	2.51	0.46
2:H:391:ALA:HB3	2:H:407:ILE:HB	1.96	0.46
2:F:316:HIS:CD2	2:F:316:HIS:N	2.84	0.46
1:C:29:GLY:HA2	3:C:600:GTP:O1A	2.16	0.46
2:H:101:ILE:HG22	2:H:118:VAL:HG13	1.98	0.46
2:H:304:GLU:OE1	2:H:323:ASN:ND2	2.36	0.46
1:C:75:ARG:CZ	1:C:76:TYR:HE1	2.29	0.46
1:E:109:MET:O	1:E:113:LEU:HD12	2.15	0.46
2:F:375:ASN:HB2	2:F:380:VAL:HG21	1.97	0.46
2:B:136:PHE:HZ	2:B:254:ILE:HG13	1.81	0.46
1:G:108:GLU:OE2	2:H:420:ARG:HD3	2.15	0.46
1:G:138:PRO:HG3	1:G:159:PRO:HB3	1.98	0.46
1:C:108:GLU:OE1	2:D:420:ARG:NH1	2.49	0.45
2:D:372:ARG:HG2	2:D:382:VAL:CG1	2.46	0.45
1:C:132:LEU:HD23	1:C:133:PRO:HD2	1.97	0.45
1:C:34:ILE:HD13	1:C:67:VAL:HG11	1.98	0.45
2:F:125:TYR:HB3	2:F:127:TYR:HE1	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:88:ASP:O	1:G:121:VAL:HB	2.17	0.45
2:H:326:VAL:HB	2:H:339:LEU:HB2	1.97	0.45
2:B:124:ILE:HD11	2:B:237:VAL:HG21	1.98	0.45
2:F:370:GLU:HB3	2:F:384:VAL:HG22	1.98	0.45
2:F:71:LEU:HD13	2:F:405:LEU:HD13	1.97	0.45
1:G:103:VAL:CG2	2:H:41:LEU:HB3	2.46	0.45
1:A:122:PRO:HG3	1:A:154:PRO:HG2	1.98	0.45
2:F:64:PHE:O	2:F:66:ASP:N	2.50	0.45
1:C:115:HIS:CE1	1:C:117:ASN:HB2	2.52	0.45
2:H:102:CYS:HB3	2:H:103:SER:H	1.62	0.45
1:C:31:THR:OG1	1:C:50:THR:OG1	2.35	0.45
2:D:217:THR:HG1	2:D:264:PRO:HG2	1.82	0.45
2:D:337:TRP:CE3	2:D:339:LEU:HD13	2.51	0.45
2:B:351:MET:O	2:B:361:ALA:N	2.43	0.45
2:H:240:GLU:HA	2:H:263:THR:HG23	1.99	0.45
1:G:103:VAL:HG21	2:H:41:LEU:HB3	1.98	0.45
2:B:268:ALA:HB3	2:B:280:THR:HB	1.98	0.44
2:B:41:LEU:CG	2:B:419:PRO:HG3	2.46	0.44
1:G:31:THR:HG23	1:G:69:ASP:OD2	2.18	0.44
1:E:21:LEU:HG	1:E:23:VAL:HG13	1.98	0.44
2:B:324:ASP:OD1	2:B:344:HIS:HA	2.18	0.44
1:A:136:MET:HA	1:A:137:PRO:HD3	1.84	0.44
1:E:100:LEU:HA	1:E:100:LEU:HD12	1.68	0.44
1:E:101:ARG:HD3	2:F:399:ARG:HB2	2.00	0.44
2:F:70:ARG:HG2	2:F:83:TRP:O	2.18	0.44
1:E:136:MET:HA	1:E:137:PRO:HD3	1.75	0.44
2:F:392:LEU:HD22	2:F:404:LEU:HD11	1.98	0.44
1:C:60:LYS:NZ	1:C:173:ASP:OD1	2.47	0.44
2:D:223:LYS:O	2:D:273:LEU:N	2.34	0.44
2:F:306:GLN:HG3	2:F:322:MET:HB2	1.99	0.44
2:H:57:CYS:HB3	2:H:74:ALA:HB3	1.99	0.44
2:D:341:LEU:HA	2:D:342:PRO:HD3	1.79	0.44
2:F:385:SER:OG	2:F:389:VAL:HG23	2.18	0.44
2:H:301:ILE:HD11	2:H:333:GLY:HA2	2.00	0.44
2:H:41:LEU:CD2	2:H:419:PRO:HG3	2.48	0.44
1:E:75:ARG:NH2	1:E:76:TYR:HE1	2.16	0.44
2:D:74:ALA:HB1	2:D:98:PRO:CG	2.42	0.43
1:E:163:LEU:HD23	1:E:163:LEU:HA	1.58	0.43
1:E:103:VAL:HG11	2:F:43:ALA:HA	2.00	0.43
1:A:92:PHE:HB3	1:A:125:TYR:CD1	2.53	0.43
2:B:57:CYS:HA	2:B:101:ILE:HG23	2.00	0.43
2:H:262:ILE:HG21	2:H:289:TYR:CE2	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:357:ARG:H	2:H:357:ARG:HG3	1.32	0.43
1:C:52:GLY:HA2	1:C:76:TYR:CD2	2.53	0.43
2:D:301:ILE:HG21	2:D:329:TYR:CE1	2.53	0.43
1:E:75:ARG:H	1:E:75:ARG:HG2	1.33	0.43
1:A:81:GLU:HA	1:A:84:TYR:CD2	2.54	0.43
2:B:313:LEU:HB2	2:B:316:HIS:O	2.18	0.43
2:B:43:ALA:HB3	2:B:415:ILE:O	2.18	0.43
2:B:97:THR:HA	2:B:98:PRO:HD3	1.77	0.43
2:H:244:ILE:HD12	2:H:291:ILE:HD12	2.00	0.43
2:B:140:PRO:HB3	2:B:213:THR:CG2	2.48	0.43
2:D:244:ILE:HD12	2:D:291:ILE:HD12	1.99	0.43
1:A:36:ARG:HA	1:A:36:ARG:HD3	1.88	0.43
2:H:111:PRO:HB2	2:H:113:LEU:CB	2.49	0.43
2:H:265:ALA:HB2	2:H:284:ARG:HG2	2.00	0.43
2:H:46:ASP:HA	2:H:47:PRO:HD2	1.77	0.43
1:A:30:LYS:N	3:A:600:GTP:O1B	2.27	0.43
2:B:221:VAL:CG1	2:B:233:SER:HB2	2.49	0.43
2:B:366:LEU:HD12	2:B:370:GLU:HB2	1.99	0.43
1:C:22:VAL:HG12	1:C:30:LYS:HD2	2.01	0.43
1:E:136:MET:HB3	1:E:141:ILE:HG13	2.01	0.43
2:B:58:VAL:HG22	2:B:73:ILE:HG23	2.01	0.43
1:C:161:ASN:HB3	1:C:166:GLU:HB3	2.01	0.43
1:E:22:VAL:HG22	1:E:91:VAL:HB	2.00	0.43
2:F:267:ILE:HG22	2:F:281:VAL:HA	2.01	0.43
2:F:298:GLN:O	2:F:300:ILE:HD12	2.19	0.43
2:F:345:ILE:HG21	2:F:348:MET:HE2	2.00	0.43
2:D:289:TYR:HD1	2:D:300:ILE:HD12	1.84	0.43
2:B:222:VAL:HA	2:B:269:VAL:HG11	2.00	0.42
2:B:351:MET:HB3	2:B:361:ALA:HB3	2.01	0.42
2:D:131:ARG:HA	2:D:132:PRO:HD3	1.71	0.42
1:G:108:GLU:CD	2:H:420:ARG:HH11	2.22	0.42
2:D:136:PHE:HE2	2:D:253:ALA:N	2.17	0.42
1:E:129:LYS:HG2	3:E:600:GTP:C6	2.54	0.42
1:E:23:VAL:C	1:E:30:LYS:HD3	2.39	0.42
2:F:219:MET:HG3	2:F:237:VAL:HG22	2.01	0.42
1:G:119:ARG:HE	1:G:119:ARG:HB2	1.63	0.42
2:D:234:CYS:HB3	2:D:247:LEU:O	2.20	0.42
1:E:113:LEU:HD23	1:E:153:ARG:CZ	2.50	0.42
2:F:351:MET:HB2	2:F:363:ILE:HD11	2.00	0.42
1:C:37:LEU:HB3	1:C:58:VAL:HG11	2.00	0.42
2:F:325:VAL:HG13	5:F:1427:PB:PB	1.63	0.42
2:F:371:VAL:HB	2:F:383:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:92:HIS:NE2	2:F:130:LEU:HD11	2.34	0.42
1:C:31:THR:HG23	1:C:69:ASP:OD2	2.19	0.42
1:C:22:VAL:HG22	1:C:91:VAL:HB	2.00	0.42
1:G:77:ARG:C	1:G:79:LEU:H	2.23	0.42
2:H:98:PRO:HA	2:H:120:ALA:HB2	2.01	0.42
2:B:134:TYR:CE2	2:B:252:THR:HA	2.55	0.42
1:C:161:ASN:O	1:C:165:GLY:N	2.50	0.42
1:A:26:ASP:OD1	2:B:399:ARG:HD2	2.19	0.42
2:D:288:LEU:HG	2:D:303:LEU:HD11	2.01	0.42
2:F:136:PHE:CZ	2:F:254:ILE:HG13	2.54	0.42
2:F:97:THR:HA	2:F:98:PRO:HD3	1.71	0.42
2:B:351:MET:HG3	2:B:394:PHE:CD2	2.55	0.42
2:D:76:GLU:C	2:D:78:ARG:H	2.22	0.42
2:D:97:THR:HA	2:D:98:PRO:HD3	1.66	0.42
2:F:291:ILE:HG12	2:F:296:LEU:HA	2.01	0.42
2:F:320:GLY:HA3	2:F:348:MET:HE2	2.01	0.42
1:E:101:ARG:NH1	2:F:399:ARG:HB2	2.34	0.42
1:G:97:ALA:HB1	1:G:134:VAL:HG23	2.01	0.42
2:D:280:THR:HG21	2:D:317:VAL:HG21	2.01	0.42
1:E:137:PRO:HD2	1:E:140:GLU:HB3	2.02	0.42
2:F:134:TYR:CD1	2:F:135:LYS:N	2.88	0.42
2:D:301:ILE:HD11	2:D:333:GLY:HA2	2.01	0.41
2:D:320:GLY:HA3	2:D:348:MET:CE	2.49	0.41
2:D:71:LEU:HD13	2:D:405:LEU:HD13	2.02	0.41
2:H:134:TYR:CD1	2:H:135:LYS:N	2.88	0.41
2:B:139:PRO:HA	2:B:140:PRO:HD3	1.89	0.41
2:B:387:ASN:CG	2:B:410:SER:HB3	2.39	0.41
2:D:122:SER:HB2	2:D:137:VAL:HG13	2.02	0.41
1:A:91:VAL:HG22	1:A:124:LEU:HD23	2.02	0.41
2:B:40:TRP:HB3	2:B:416:LYS:HB3	2.02	0.41
1:C:136:MET:HB3	1:C:136:MET:HE3	1.86	0.41
1:A:94:VAL:HG21	1:A:141:ILE:HG21	2.01	0.41
2:H:59:HIS:NE2	2:H:103:SER:HB3	2.35	0.41
2:B:327:HIS:CG	2:B:335:LYS:HE3	2.56	0.41
2:B:396:ARG:NH2	2:B:399:ARG:HA	2.35	0.41
1:C:103:VAL:HG21	2:D:41:LEU:HB3	2.03	0.41
2:H:111:PRO:C	2:H:113:LEU:HA	2.40	0.41
2:H:97:THR:HA	2:H:98:PRO:HD3	1.86	0.41
2:B:258:ILE:HD13	2:B:291:ILE:HD13	2.03	0.41
2:B:337:TRP:CE3	2:B:339:LEU:HD13	2.56	0.41
2:H:370:GLU:OE2	2:H:372:ARG:NH2	2.54	0.41
2:D:118:VAL:O	2:D:124:ILE:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:30:LYS:O	1:G:34:ILE:HG13	2.21	0.41
2:D:320:GLY:HA3	2:D:348:MET:HE2	2.02	0.41
2:B:405:LEU:HA	2:B:405:LEU:HD23	1.86	0.41
1:C:103:VAL:CG1	2:D:43:ALA:HA	2.46	0.41
2:D:80:LEU:HD23	2:D:94:LEU:HD11	2.02	0.41
2:H:113:LEU:N	2:H:114:PRO:CD	2.83	0.41
2:H:81:LYS:HD3	2:H:88:LYS:NZ	2.36	0.41
1:A:25:LEU:HA	1:A:25:LEU:HD23	1.91	0.41
2:D:43:ALA:HB3	2:D:415:ILE:O	2.20	0.41
2:F:303:LEU:CD2	2:F:319:VAL:HG21	2.51	0.41
2:H:145:THR:HG22	2:H:146:GLU:H	1.86	0.41
2:H:312:ARG:O	2:H:350:ARG:NH1	2.54	0.41
1:C:17:LYS:HB3	1:C:17:LYS:HE3	1.71	0.41
1:G:96:SER:HB3	1:G:136:MET:H	1.86	0.41
2:H:351:MET:HB3	2:H:361:ALA:HB3	2.03	0.41
2:F:370:GLU:HA	2:F:384:VAL:HA	2.03	0.40
1:A:177:GLU:OE1	1:A:178:ARG:NH2	2.53	0.40
2:D:266:MET:HG2	2:D:282:ALA:HB3	2.03	0.40
2:D:288:LEU:HD11	2:D:319:VAL:HG11	2.04	0.40
1:E:28:SER:HB2	1:E:93:VAL:HG12	2.03	0.40
1:G:100:LEU:HD12	1:G:100:LEU:HA	1.87	0.40
1:G:28:SER:HA	1:G:95:ASP:HB2	2.04	0.40
2:B:246:ILE:O	2:B:255:VAL:N	2.42	0.40
2:F:374:TYR:CE1	2:F:379:LEU:HB2	2.57	0.40
2:B:349:GLN:NE2	2:B:392:LEU:O	2.48	0.40
1:C:52:GLY:HA2	1:C:76:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	164/169 (97%)	155 (94%)	9 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	164/169 (97%)	152 (93%)	12 (7%)	0	100	100
1	E	164/169 (97%)	153 (93%)	11 (7%)	0	100	100
1	G	164/169 (97%)	154 (94%)	10 (6%)	0	100	100
2	B	329/425 (77%)	294 (89%)	34 (10%)	1 (0%)	50	92
2	D	299/425 (70%)	267 (89%)	31 (10%)	1 (0%)	50	92
2	F	303/425 (71%)	273 (90%)	29 (10%)	1 (0%)	50	92
2	H	321/425 (76%)	293 (91%)	28 (9%)	0	100	100
All	All	1908/2376 (80%)	1741 (91%)	164 (9%)	3 (0%)	56	94

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	209	PRO
2	F	65	GLY
2	D	65	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	132/142 (93%)	128 (97%)	4 (3%)	53	87
1	C	138/142 (97%)	136 (99%)	2 (1%)	78	94
1	E	135/142 (95%)	126 (93%)	9 (7%)	23	67
1	G	137/142 (96%)	132 (96%)	5 (4%)	47	84
2	B	243/352 (69%)	224 (92%)	19 (8%)	18	59
2	D	214/352 (61%)	196 (92%)	18 (8%)	16	55
2	F	221/352 (63%)	210 (95%)	11 (5%)	34	77
2	H	243/352 (69%)	225 (93%)	18 (7%)	20	62
All	All	1463/1976 (74%)	1377 (94%)	86 (6%)	28	72

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	119	ARG
1	A	178	ARG
1	A	180	SER
2	B	55	THR
2	B	70	ARG
2	B	78	ARG
2	B	87	GLN
2	B	91	GLU
2	B	101	ILE
2	B	104	TYR
2	B	105	ILE
2	B	108	ASN
2	B	130	LEU
2	B	148	GLN
2	B	213	THR
2	B	245	LEU
2	B	263	THR
2	B	301	ILE
2	B	306	GLN
2	B	312	ARG
2	B	316	HIS
2	B	343	CYS
1	C	56	ASP
1	C	178	ARG
2	D	60	THR
2	D	70	ARG
2	D	83	TRP
2	D	86	THR
2	D	124	ILE
2	D	125	TYR
2	D	128	ARG
2	D	129	ASN
2	D	135	LYS
2	D	136	PHE
2	D	262	ILE
2	D	306	GLN
2	D	311	VAL
2	D	313	LEU
2	D	316	HIS
2	D	322	MET
2	D	343	CYS
2	D	382	VAL

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Mol	Chain	Res	Type
1	E	38	LYS
1	E	75	ARG
1	E	78	THR
1	E	94	VAL
1	E	119	ARG
1	E	124	LEU
1	E	134	VAL
1	E	178	ARG
1	E	179	LEU
2	F	62	ASN
2	F	86	THR
2	F	130	LEU
2	F	134	TYR
2	F	221	VAL
2	F	296	LEU
2	F	316	HIS
2	F	317	VAL
2	F	343	CYS
2	F	421	THR
2	F	425	GLU
1	G	64	THR
1	G	75	ARG
1	G	78	THR
1	G	119	ARG
1	G	178	ARG
2	H	48	VAL
2	H	52	SER
2	H	55	THR
2	H	70	ARG
2	H	94	LEU
2	H	96	ASP
2	H	104	TYR
2	H	108	ASN
2	H	128	ARG
2	H	130	LEU
2	H	143	VAL
2	H	145	THR
2	H	303	LEU
2	H	316	HIS
2	H	343	CYS
2	H	354	THR
2	H	357	ARG

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Mol	Chain	Res	Type
2	H	425	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	257	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 22 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GTP	A	600	4	34,34,34	1.09	2 (5%)	52,54,54	2.69	8 (15%)
3	GTP	C	600	4	34,34,34	1.08	2 (5%)	52,54,54	2.66	10 (19%)
3	GTP	E	600	4	34,34,34	1.15	2 (5%)	52,54,54	3.36	10 (19%)
3	GTP	G	600	4	34,34,34	1.11	2 (5%)	52,54,54	2.53	10 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	600	4	-	0/22/38/38	0/3/3/3
3	GTP	C	600	4	-	0/22/38/38	0/3/3/3
3	GTP	E	600	4	-	0/22/38/38	0/3/3/3
3	GTP	G	600	4	-	0/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	GTP	C2-N3	4.39	1.38	1.33
3	E	600	GTP	C2-N3	4.17	1.38	1.33
3	G	600	GTP	C2-N3	3.65	1.38	1.33
3	C	600	GTP	C2-N3	3.23	1.37	1.33
3	G	600	GTP	C5-N7	-2.81	1.34	1.38
3	C	600	GTP	C5-N7	-2.28	1.35	1.38
3	E	600	GTP	C5-N7	-2.22	1.35	1.38
3	A	600	GTP	C5-N7	-2.12	1.35	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	GTP	C6-C5-N7	-20.86	131.33	134.14
3	A	600	GTP	C6-C5-N7	-15.61	132.04	134.14
3	C	600	GTP	C6-C5-N7	-15.16	132.10	134.14
3	G	600	GTP	C6-C5-N7	-13.94	132.26	134.14
3	A	600	GTP	C5-C4-N3	-4.86	120.47	126.07
3	E	600	GTP	PA-O3A-PB	-4.57	119.27	131.93
3	E	600	GTP	C5-C4-N3	-4.52	120.86	126.07
3	A	600	GTP	PA-O3A-PB	-4.42	119.70	131.93
3	G	600	GTP	PB-O3B-PG	-4.38	119.80	131.93
3	C	600	GTP	PA-O3A-PB	-4.25	120.16	131.93
3	G	600	GTP	C5-C4-N3	-4.24	121.19	126.07
3	E	600	GTP	O3A-PB-O3B	4.13	110.06	101.66
3	C	600	GTP	PB-O3B-PG	-3.92	121.07	131.93
3	G	600	GTP	PA-O3A-PB	-3.90	121.13	131.93
3	A	600	GTP	N3-C4-N9	3.86	132.57	126.91
3	A	600	GTP	C2-N3-C4	3.85	119.92	115.30
3	E	600	GTP	N3-C4-N9	3.73	132.38	126.91
3	G	600	GTP	C2-N3-C4	3.66	119.69	115.30
3	C	600	GTP	C5-C4-N3	-3.39	122.16	126.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	GTP	PB-O3B-PG	-3.32	122.74	131.93
3	E	600	GTP	C2'-C3'-C4'	-3.28	96.10	102.64
3	A	600	GTP	O3A-PB-O3B	3.18	108.13	101.66
3	G	600	GTP	O3A-PB-O3B	3.10	107.96	101.66
3	C	600	GTP	N3-C4-N9	3.09	131.44	126.91
3	E	600	GTP	C2-N3-C4	3.06	118.97	115.30
3	G	600	GTP	N3-C4-N9	3.05	131.39	126.91
3	C	600	GTP	O3A-PB-O3B	3.00	107.77	101.66
3	C	600	GTP	C2'-C3'-C4'	-2.91	96.82	102.64
3	C	600	GTP	C2-N3-C4	2.85	118.72	115.30
3	E	600	GTP	O4'-C1'-C2'	-2.72	102.73	106.69
3	E	600	GTP	O3'-C3'-C4'	-2.66	103.24	111.07
3	C	600	GTP	N2-C2-N1	2.66	120.67	117.82
3	E	600	GTP	O2'-C2'-C1'	2.59	119.69	111.49
3	G	600	GTP	O4'-C1'-N9	-2.56	102.53	108.10
3	G	600	GTP	C3'-C2'-C1'	2.43	104.73	100.92
3	C	600	GTP	C8-N9-C4	2.42	108.92	106.96
3	G	600	GTP	C5'-C4'-C3'	-2.11	106.72	115.19
3	A	600	GTP	O4'-C1'-N9	-2.07	103.60	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	166/169 (98%)	0.08	1 (0%) 86 53	9, 35, 61, 85	0
1	C	166/169 (98%)	0.05	0 100 100	1, 4, 33, 48	0
1	E	166/169 (98%)	0.06	0 100 100	1, 8, 39, 66	0
1	G	166/169 (98%)	0.10	1 (0%) 86 53	8, 24, 51, 60	0
2	B	333/425 (78%)	-0.02	0 100 100	1, 16, 50, 81	0
2	D	307/425 (72%)	0.25	11 (3%) 41 14	2, 44, 96, 105	0
2	F	309/425 (72%)	0.23	3 (0%) 79 42	1, 37, 92, 120	0
2	H	325/425 (76%)	0.01	0 100 100	1, 16, 49, 77	0
All	All	1938/2376 (81%)	0.10	16 (0%) 83 47	1, 21, 83, 120	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	235	LEU	3.8
2	F	216	ILE	3.2
2	F	133	TYR	3.1
2	D	246	ILE	2.6
2	D	63	LEU	2.6
2	D	80	LEU	2.5
1	A	65	PHE	2.3
2	D	258	ILE	2.3
2	D	219	MET	2.3
2	D	126	ILE	2.3
2	D	94	LEU	2.3
2	D	260	VAL	2.1
2	D	244	ILE	2.1
2	F	291	ILE	2.1
1	G	179	LEU	2.1
2	D	116	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	G	601	1/1	0.24	2.00	15,15,15,15	0
4	MG	E	601	1/1	0.23	1.75	6,6,6,6	0
4	MG	C	601	1/1	0.28	1.40	1,1,1,1	0
4	MG	A	601	1/1	0.22	0.87	29,29,29,29	0
5	PB	H	1427	1/1	0.28	0.35	16,16,16,16	1
3	GTP	C	600	32/32	0.24	0.17	1,3,4,4	0
3	GTP	E	600	32/32	0.22	-0.06	5,8,14,17	0
3	GTP	A	600	32/32	0.18	-0.20	29,35,46,48	0
3	GTP	G	600	32/32	0.20	-0.39	15,19,25,26	0
5	PB	A	1181	1/1	0.19	-0.39	170,170,170,170	1
5	PB	H	1426	1/1	0.16	-0.50	35,35,35,35	1
5	PB	F	1427	1/1	0.18	-0.58	23,23,23,23	1
5	PB	A	1182	1/1	0.18	-0.63	112,112,112,112	1
5	PB	B	1428	1/1	0.12	-1.26	12,12,12,12	1
5	PB	D	1426	1/1	0.10	-1.44	35,35,35,35	1
5	PB	D	1427	1/1	0.09	-1.53	79,79,79,79	1
5	PB	G	1181	1/1	0.12	-1.66	106,106,106,106	1
5	PB	D	1428	1/1	0.05	-1.81	140,140,140,140	1
5	PB	H	1428	1/1	0.11	-1.83	89,89,89,89	1
5	PB	F	1426	1/1	0.08	-1.95	83,83,83,83	1
5	PB	B	1429	1/1	0.08	-2.00	66,66,66,66	1
5	PB	B	1426	1/1	0.14	-2.16	33,33,33,33	1
5	PB	B	1427	1/1	0.10	-2.27	85,85,85,85	1
5	PB	H	1429	1/1	0.08	-2.84	84,84,84,84	1
5	PB	E	1181	1/1	0.09	-2.90	120,120,120,120	1
5	PB	F	1428	1/1	0.08	-4.26	83,83,83,83	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.